

# Certificate of Analysis

[www.tocris.com](http://www.tocris.com)

**Product Name:** PF 998425

**Catalog No.:** 3923

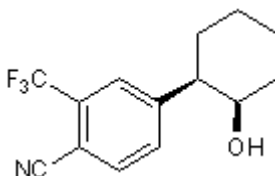
**Batch No.:** 1

**CAS Number:** 1076225-27-8

**IUPAC Name:** 4-((1*R*,2*R*)-2-Hydroxycyclohexyl)-2(trifluoromethyl)benzonitrile

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>14</sub>H<sub>14</sub>F<sub>3</sub>NO  
**Batch Molecular Weight:** 269.26  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
 ethanol to 100 mM  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 98.0% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Optical Rotation:** [α]<sub>D</sub> = -66.6 (Concentration = 1, Solvent = Chloroform)  
**Microanalysis:**

	Carbon Hydrogen Nitrogen		
Theoretical	62.45	5.24	5.2
Found	62.34	5.22	5.18

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

## Product Information

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### Description:

Selective non-steroidal androgen receptor (AR) antagonist (IC<sub>50</sub> values are 26 nM and 90 nM in AR binding assays and cellular assays respectively). Displays low affinity for progesterone receptor (IC<sub>50</sub> > 10 µM). Active in vivo.

### Physical and Chemical Properties:

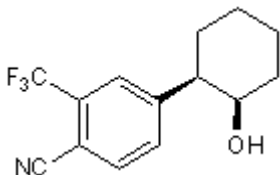
Batch Molecular Formula: C<sub>14</sub>H<sub>14</sub>F<sub>3</sub>NO

Batch Molecular Weight: 269.26

Physical Appearance: White solid

**Minimum Purity:** >98%

### Batch Molecular Structure:



**Storage:** Store at +4°C

### Solubility & Usage Info:

DMSO to 100 mM

ethanol to 100 mM

### Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

**SOLIDS:** Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

**SOLUTIONS:** We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

### References:

Li *et al* (2008) Rational design and synthesis of 4-((1*R*,2*R*)-2-hydroxycyclohexyl)-2(trifluoromethyl)benzonitrile (PF-998425), a novel, nonsteroidal androgen receptor antagonist devoid of phototoxicity for dermatological indications. *J.Med.Chem.* **51** 7010. PMID: 18921992.

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